# Trustworthy Machine Learning and Robust Artificial Intelligence

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# **Outline**

- Motivation: Why Trustworthy and Robust AI?
- Part 1: Trustworthy Machine Learning
- Part 2: Robust Artificial Intelligence
  - Part 2A: Robust Autonomous Al Systems
  - Part 2B: Robust Human/Al Teams

# **Self-Driving Cars**



Credit: delphi.com<sup>Science</sup> Nigeria Al Bootcamp

Credit: Tesla Motors

# **Automated Stock Trading**



CADE METZ BUSINESS 01.25.16 7:00 AM

THE RISE OF THE ARTIFICIALLY INTELLIGENT HEDGE FUND



Oct 3rd 2019

### The rise of the financial machines

Forget Gordon Gekko. Computers increasingly call the shots in financial markets



# **Autonomous Weapons**

### Northroop Grumman X-47B



Credit: Wikipedia

### UK Brimstone Anti-Armor Weapon



Credit: Duch.seb - Own work, CC BY-SA 3.0

Samsung SGR-1



Credit: AFP/Getty Images

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- Part 1: Trustworthy Machine Learning
- Part 2: Robust Artificial Intelligence
  - Part 2A: Robust Autonomous AI Systems
  - Part 2B: Robust Human/Al Teams

# Part 1: Trustworthy Machine Learning

Threats to Machine Learning Performance

- Assumption of Independent and Identically Distributed (iid) Data
- Closed World Assumption: The class labels are mutually-exclusive and exhaustive
- Adversarial Attacks

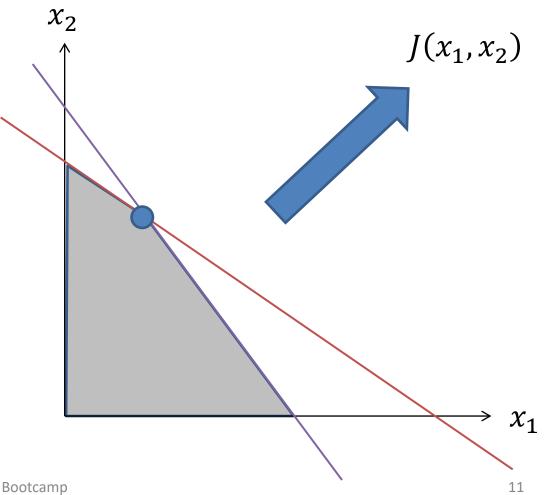
How can we be confident in the accuracy of a machine learning system?

- 1. Robustness by Construction
- 2. Self-Model of Competence
  - Calibrated Probabilities
  - Reject Option
- 3. Monitoring for Data Shift

# Robustness by Construction: Minimaxing Against an Adversary

- Many AI reasoning problems can be formulated as optimization problems
- $\bullet \max_{x_1,x_2} J(x_1,x_2)$
- subject to

$$ax_1 + bx_2 \le r$$
  
$$cx_1 + dx_2 \le s$$



# **Uncertainty in the constraints**

- $\bullet \max_{x_1,x_2} J(x_1,x_2)$
- subject to

$$ax_1 + bx_2 \le r$$
  
$$cx_1 + dx_2 \le s$$

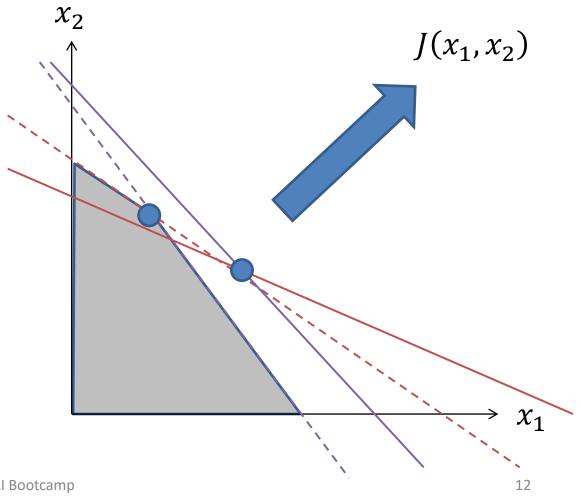
Define uncertainty regions

$$a \in U_a$$

$$b \in U_b$$

$$\dots$$

$$s \in U_s$$



# Minimax against the uncertainty sets

- $\max_{x_1,x_2} \min_{a,b,c,d,r,s} J(x_1,x_2;a,b,c,d,r,s)$
- subject to

$$ax_1 + bx_2 \le r$$

$$cx_1 + dx_2 \le s$$

$$a \in U_a$$

$$b \in U_b$$
...
$$s \in U_s$$

Problem: Solutions can be too conservative

# Solution: Impose a Budget on the Adversary

- $\max_{x_1,x_2} \min_{\delta_a,\dots,\delta_s} J(x_1,x_2;\delta_a,\dots,\delta_s)$
- subject to

$$(a + \delta_a)x_1 + (b + \delta_b)x_2 \leq (r + \delta_r)$$

$$(c + \delta_c)x_1 + (d + \delta_d)x_2 \leq (s + \delta_s)$$

$$\delta_a \in U_a$$

$$\delta_b \in U_b$$
...
$$\delta_s \in U_s$$

$$\sum |\delta_i| \leq B$$

Bertsimas, et al.; Ben-Tal, Nemirovski, & El Ghaoui (2009)

# **Robustness By Construction: Classification**

- Goal: Train Deep Networks so that they are guaranteed to be robust to adversarial perturbations in the test queries
  - Measured as bound on the size of the Manhattan  $(\ell_1)$  or Euclidean  $(\ell_2)$  norm of the perturbation
- Approach for Linear Classifiers (e.g., linear SVM)
  - Minimax against an adversary who can perturb training point  $x_i$  by an  $\ell_2$  perturbation  $\delta_i$ ,  $i=1,\ldots,n$
  - This turns out to be equivalent to  $\ell_2$  regularization with a total budget  $\lambda = \sum_i \|\delta_i\|$
  - During training, find  $\theta$  to minimize  $\sum_{i} L(y_i, f(x_i, \theta)) + \lambda \|\theta\|$
- Approach for Deep Learning: Stability Training with Noise (STN)
  - Li, Chen, Wang & Carin, 2019, arXiv 1809.03113v5
  - Find  $\theta$  to minimize

$$\sum_{i} L(y_i, f(x_i, \theta)) + \lambda D(f(x_i), f(x_i + \delta_i)) \text{ where } \delta_i \sim N(0, \sigma^2 I)$$

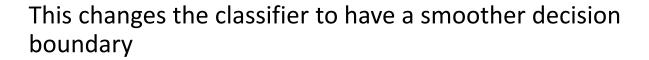
$$-D(f(x_i), f(x_i + \delta_i)) = \sum_j P(\hat{y} = j | x_i) \log P(\hat{y} = j | x_i + \delta_i)$$
 is the cross-entropy loss

# **Stability Training with Noise**

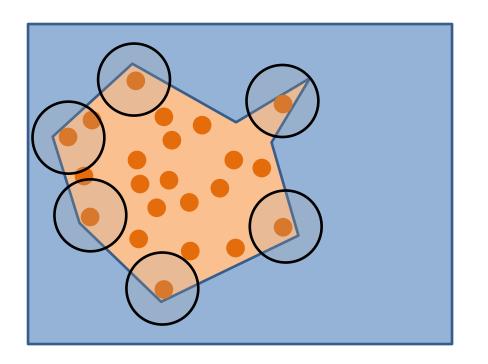
 Testing: Stability testing. Measure the distribution of predictions computed with Gaussian perturbations and predict the class with highest probability

$$p_{ij} = \frac{1}{M} \sum_{m=1}^{M} \mathbb{I} [\hat{f}(x_i + \delta_i) = j] \quad \delta_i \sim N(0, \sigma^2 I)$$

$$\hat{f}_{stab}(x_i) = \arg\max_{j} p_{ij}$$



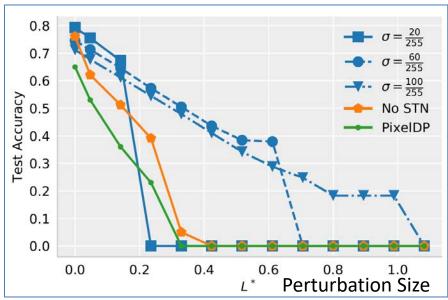
Note that this is done on the test set. It provides a formal guarantee that there are no adversarial examples within a specified radius. First method that can give a non-trivial guarantee for ImageNet



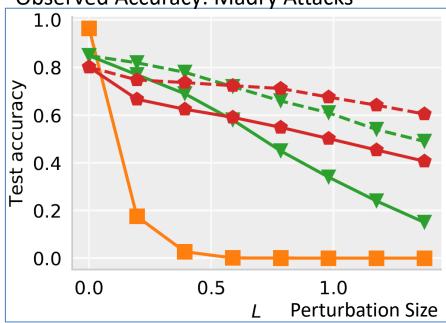
# **Stability Training with Noise**

- Top plot: Theoretical Guarantee.
   Accuracy is ≥ plotted value with probability 0.95.
  - Key: STN, PixelDP (Lecuyer et al. 2018)
- Bottom plot: Experimental Accuracy. Key:
  - STN, TRADES (Zhang et al. 2019).
  - Dashes = black box (Madri attacks); solid = white box (modified Carlini & Wagner attacks)

### Guaranteed Test Accuracy: CIFAR-10



Observed Accuracy: Madry Attacks



# **Self-Model of Competence**

- Given
  - Training data  $S_{train}$
  - Learned classifier  $\hat{f}$  that outputs a probability vector  $\hat{p}$
  - Test queries  $S_{test} = \{x_1, ..., x_N\}$
- Let  $\hat{p}(x_i) = (\hat{p}_{i1}, ..., \hat{p}_{ik})$  be the predicted probabilities for  $x_i$
- Let  $p(x_i) = (p_{i1}, ..., p_{ik})$  be the true probabilities
  - includes randomness due to feature measurement error and label noise ("aleatory uncertainty")
- A classifier is well calibrated if

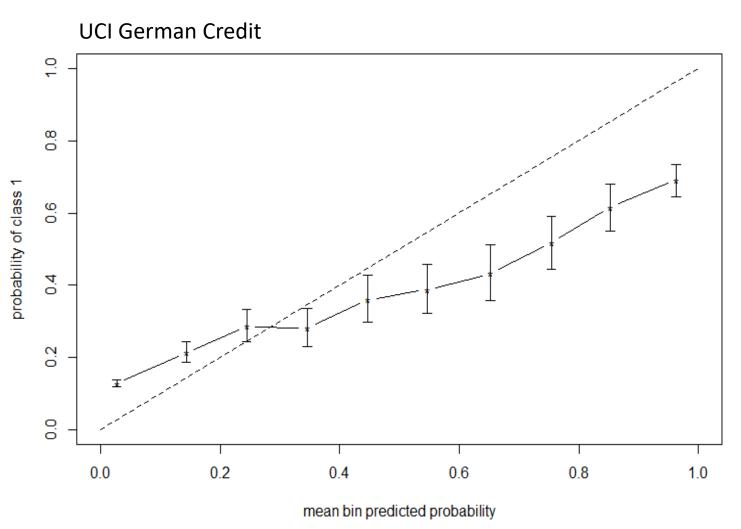
$$\hat{p}(x_i) = p(x_i)$$

Weaker condition: probability of the most likely class matches

$$\max_{j} \hat{p}_{ij} = \max_{j} p_{ij}$$

# **Evaluating Calibration Using a Reliability Diagram**

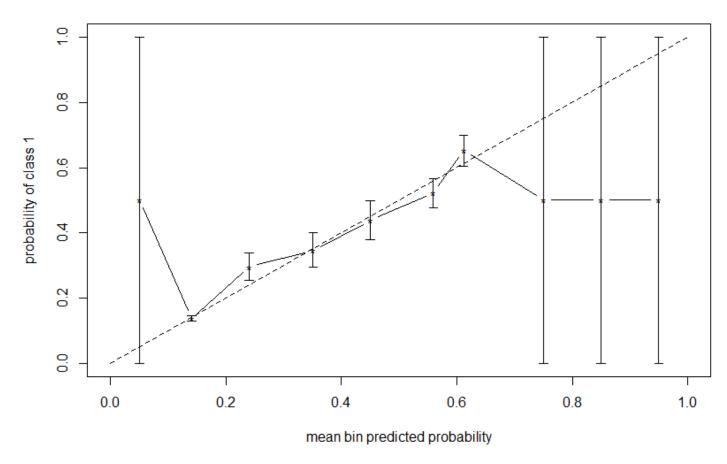
- On a labeled "calibration data set", sort  $x_i$  into bins according to  $\hat{p}_{i1}$  [0,0.1),[0.1,0.2),...
- Compute the fraction of points in each bin for which  $y_i = 1$
- Plot with confidence intervals
- Classifier: R gbm with 10,000 trees



# **Recalibration Methods**

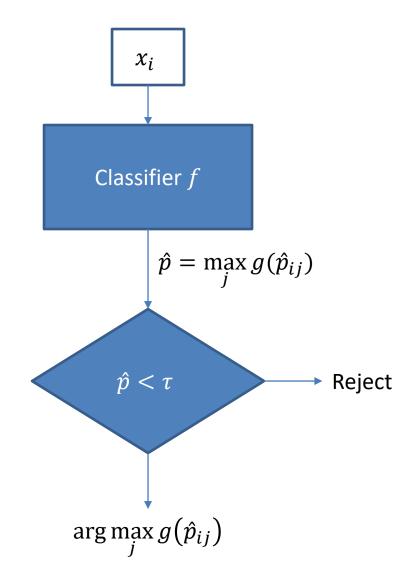
- Several techniques have been developed for fixing poor calibration by fitting a function g such that  $\tilde{p} \coloneqq g(\hat{p})$  is better calibrated
  - Platt scaling (logistic regression)
  - Isotonic regression
  - Kernel logistic regression
  - Gaussian Process regression
- Reliability Diagram after Platt scaling
  - Predicted probabilities have been rescaled into the range 0.1-0.6

### **Platt Scaling**



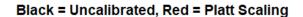
# **Using Calibrated Probabilities for Rejection**

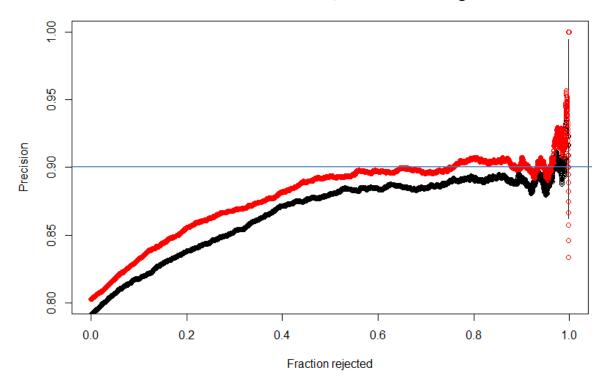
 If classifier is not confident enough, then it should reject the query

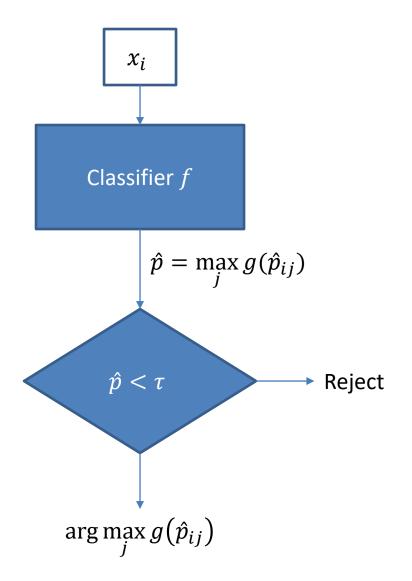


# **Using Calibrated Probabilities for Rejection**

- If classifier is not confident enough, then it should reject the query
- Rejection curve. Plot precision as a function of fraction of queries rejected (by varying  $\tau$ )







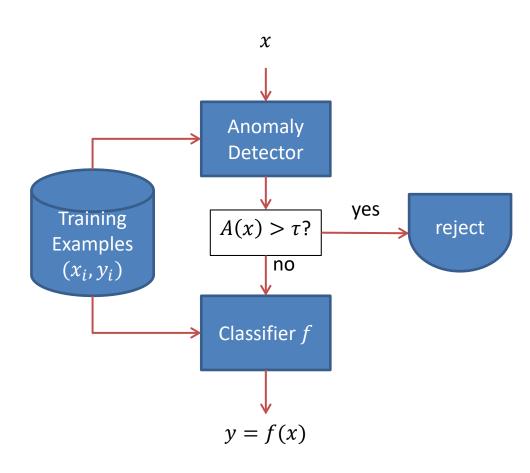
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Al Bootcamp

# **Monitoring for Data Shift and Novel Categories**

### Method 1: Anomaly Detection

- Unsupervised Anomaly Detection
- Given:
  - Training data  $S_{train}$  assumed to be drawn iid from  $P_{train}$
  - Test query x
- Decide whether x is also drawn from  $P_{train}$
- Direct method
  - Estimate  $\hat{P}_{train}$  from the training data ("density estimation")
  - Score x by "Surprise":  $A(x) = -\log \hat{P}_{train}(x)$
  - Difficulty: density estimation requires very large sample sizes in general



# **Benchmarking Practical Anomaly Detection Methods**

- Goal: Compare published algorithms on a robust collection of benchmarks
  - Previous comparisons suffered from small size and/or proprietary data sets

### Density-Based Approaches

- RKDE: Robust Kernel Density
   Estimation (Kim & Scott, 2008)
- EGMM: Ensemble Gaussian
   Mixture Model (our group)

### Quantile-Based Methods

- OCSVM: One-class SVM (Schoelkopf, et al., 1999)
- SVDD: Support Vector Data
   Description (Tax & Duin, 2004)

### Neighbor-Based Methods

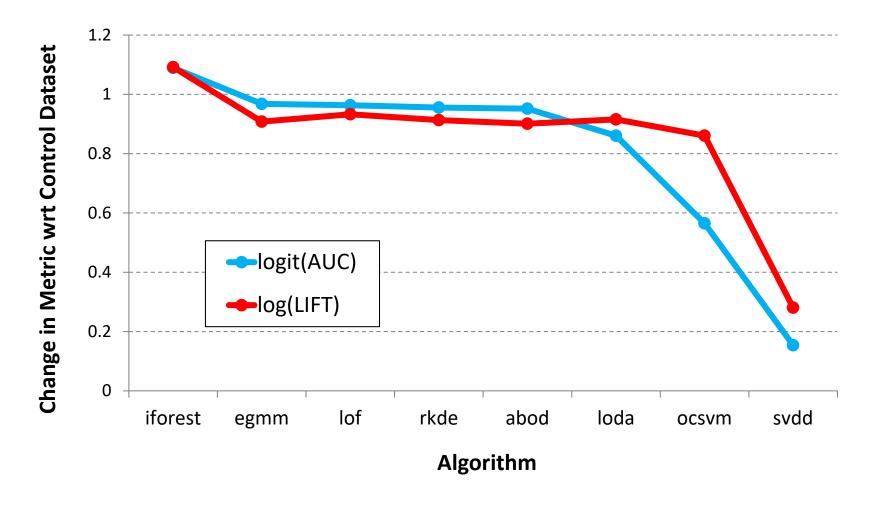
- LOF: Local Outlier Factor (Breunig, et al., 2000)
- ABOD: kNN Angle-Based Outlier
   Detector (Kriegel, et al., 2008)

### Projection-Based Methods

- IFOR: Isolation Forest (Liu, et al., 2008)
- LODA: Lightweight Online Detector of Anomalies (Pevny, 2016)

[Emmott, Das, Dietterich, Fern, Wong, 2013; KDD ODD-2013] [Emmott, Das, Dietterich, Fern, Wong. 2016; arXiv 1503.01158v2]

# **Anomaly Detection Benchmark Results**



iForest was best; quantile methods were worst; all others approximately equal

# **Anomaly Detection Challenges**

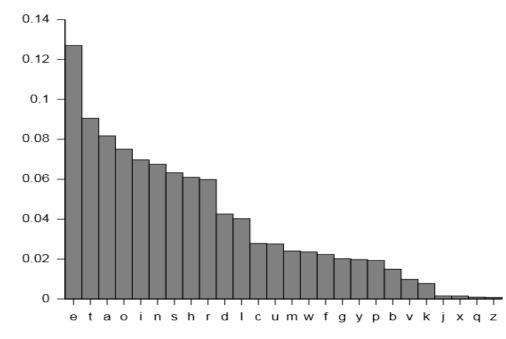
- High-dimensional spaces are inherently difficult
  - Can we assume the data live in a lower-dimensional subspace?
- Image and video data
  - Need to discover the lower-dimensional space
- Promising directions
  - Auto-encoders and generative models (VAE, RAE, BiGAN)
  - Neural Rendering Model
  - Extending existing methods to work with time series

# Data Shift Detection: Method 2: Monitor the Distribution of Predicted Classes

# Supervised classification

- On training data, measure expected class frequencies
- Detect departures from these on test data
- Mismatch can indicate a change in the class distribution or a failure in the classifier

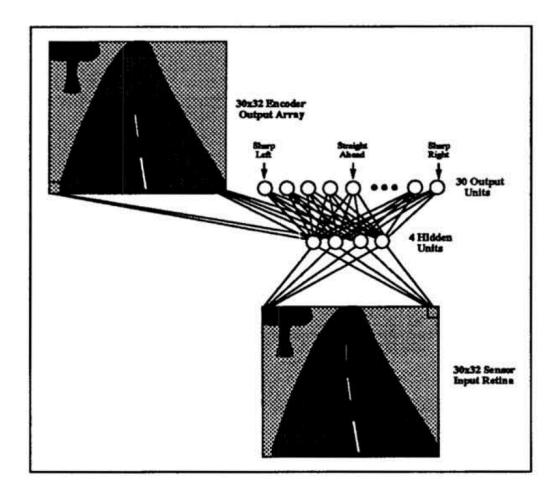
### Letter frequencies in English



Credit: Nandhp, Wikipedia

# **Method 3: Monitor Auxiliary Tasks**

- ALVINN auto-steer system
- Main task: Determine steering command
- Auxiliary task: Predict input image
- Perform both tasks with the same hidden layer information



Pomerleau, NIPS 1992

# Data Shift Detection Method 4: Two-Sample Testing

- Compare  $S_{train}$  to  $S_{test}$
- Technique 1: Two-sample Tests
  - Kernel Two-sample Test based on Maximum Mean Discrepancy (Gretton, et al.)
- Technique 2: Old-vs-New Classifier
  - Label  $S_{train}$  as class 0 "old" data
  - Label  $S_{test}$  as class 1 "new" data
  - Train a classifier and evaluate via cross-validation
  - If the classifier can do better than random guessing, then we have data shift

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  - Part 2B: Robust Human/Al Teams

# **Goal: Robust Artificial Intelligence**

- Definition: System remains safe and successful in spite of
  - Errors in the problem formulation
  - Errors in authored or learned models
  - Sensor failures
  - Changes in the system and in the world
  - Errors by human operators
  - Breakdowns in human teams
  - Cyberattack

# **High Reliability Organizations**

### **Todd LaPorte, Gene Rochlin, and Karlene Roberts**

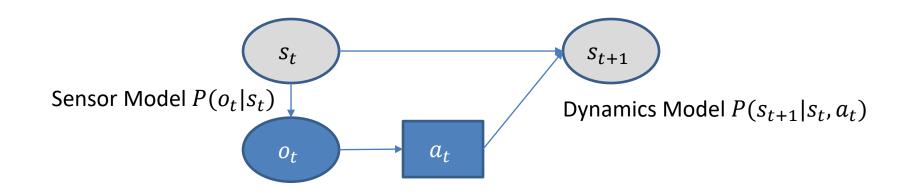
- Studied several high reliability human teams
  - Air Traffic Control
  - Nuclear power plant operations
  - Aircraft Carrier flight deck operations
- Claim: Accidents can be prevented through organizational design, culture, management, and human choices
- Impact:
  - Patient safety movement
  - Cockpit resource management

# **Properties of High Reliability Organizations**

- Preoccupation with failure
  - Fundamental belief that the system has unobserved failure modes
  - Treat anomalies and near misses as symptoms of a problem with the system
- Reluctance to simplify interpretations
  - Comprehensively understand the situation
- Sensitivity to operations
  - Maintain continuous situational awareness
- Commitment to resilience
  - Develop the capability to detect, contain, and recover from errors. Practice improvisational problem solving
- Deference to expertise
  - During a crisis, authority migrates to the person who can solve the problem, regardless of their rank

# PART 2A: AUTONOMOUS AI SYSTEMS

# **Maintain Situational Awareness**



- Maintain a probability distribution  $P(s_t)$  over the state of the system
- Collect the observations  $o_t$
- Compute updated distribution:

$$P(s_t|o_t) \propto P(o_t|s_t)P(s_t)$$

- Choose the action  $a_t$
- Predict next state distribution:

$$P(s_{t+1}|o_t, a_t) = \sum_{s_t} P(s_{t+1}|a_t, s_t) P(s_t|o_t)$$

### Methods:

- Kalman filter
- Particle filters
- Expectation propagation
- Variational approximations
- etc.

# **Detect Anomalies and Near Misses**

### **Detecting Anomalies**

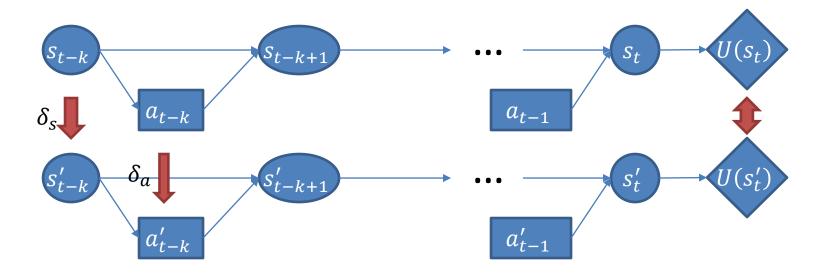
- Compute the "surprise" of the observed  $o_{t+1}$
- Predicted distribution of  $o_{t+1}$ :

$$P(o_{t+1}|o_t, a_t) = \sum_{s_{t+1}} P(s_{t+1}|o_t, a_t) P(o_{t+1}|s_{t+1})$$

Anomaly Score:

$$-\log P(o_{t+1}|o_t,a_t)$$

# **Detecting Near Misses**



- Suppose we have a utility function U(s) over states
- Counterfactual Notion: Perturb  $s_{t-k}$  and/or  $a_{t-k}$
- Near Miss:

$$U(s_t') \ll U(s_t)$$

- Detecting near misses is under-studied; requires causal model
- Should anticipate them and act to prevent them

# **Explaining Anomalies and Near Misses: Research Challenges**

- Open-ended space of hypotheses
  - Effects of exogenous variables / unknown external agents?
    - what external agents might exist and why would they be affecting our system?
  - Sensor failures and/or inadequate sensors
    - why didn't we detect the anomaly or near miss earlier?
  - Model failures (dynamics and sensor models)
    - did the system structure change? (broken pipe? stuck valve?)
- Promising work
  - Model-based diagnosis including performing information-gathering actions

# **Improvising Solutions: Finding Repairs and Workarounds**

# Approaches

- Update dynamics and sensor models and then apply planning algorithms?
- Mark aspects of the models as unreliable and seek a plan that does not depend on those aspects?
- Always plan conservatively to be robust to model errors?

## **Summary: Autonomous Al**

	Assessment
Situational Awareness	A mature methods
Detect Anomalies and Near Misses	B high-dimension, dynamics
Explain Anomalies and Near Misses	D only basic techniques
Improvise Solutions	F

#### PART 2B: AI + HUMAN TEAMS

#### Al and Human Teams

- Even very powerful AI systems will be surrounded by a human team that will determine
  - What goals to give it
  - What degree of autonomy to permit it
  - When to trust it
  - What degree of learning/adaptation to allow
- How can the combined AI + Human Team be safe and robust?
  - Reconsider each aspect of high-reliability organizations from an interactive perspective

#### **Situational Awareness: Past Failures**

- Autopilot Tunnel Vision: Aircraft autopilot not aware of air traffic control instructions
  - Co-pilot must continually update the autopilot's waypoints based on ATC interactions
  - This load increases in high-traffic/high-risk situations
  - Co-pilot loses awareness of other aspects of the system
- Autopilot Fails to Communicate Situation
  - Colgan Air 3407 crash near Buffalo
  - Autopilot was compensating for aircraft icing, but pilots were not aware of this
  - Eventually autopilot was forced to hand control back to pilots
  - Their lack of situational awareness led to crash ("decompensation failure")
- Autopilot Over-Communicates
  - Hundreds of unimportant alarms
  - Complex displays that bury important information
- Humans Misunderstand Internal State of Autonomous System
  - USS John McCain collision: team thought single slider was controlling both engines, but it was controlling only one
  - Caused ship to turn into the course of an oncoming ship

#### **Requirements for Robust Situational Awareness**

- Al system should have sufficient sensing
  - state of world including other agents
  - state of the system being controlled
  - state of its human team
- Human team and AI system should establish and maintain a shared mental model
  - Al system should reason about what the users know and do not know and communicate strategically
  - Humans need a good mental model of the AI system's beliefs about the situation
  - Al system needs to be able to explain its beliefs to humans
  - Careful design of user interface is critical

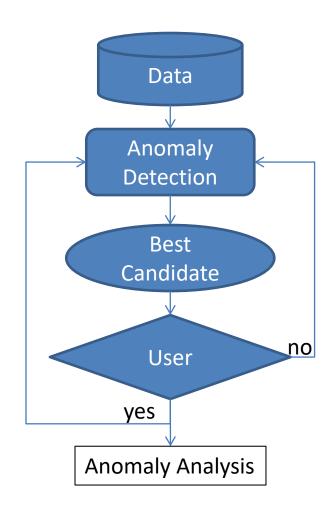
#### **Anomaly and Near Miss Detection**

- Existing methods are highly local
  - sensor readings out of standard range
  - violations of minimum separation (air-to-air, air-to-ground, car-tocar)
- Need more and better anticipation of problems
  - model the behavior of other agents (including team members)
  - project system state many steps into the future and evaluate
- Incorporate interactive anomaly detection

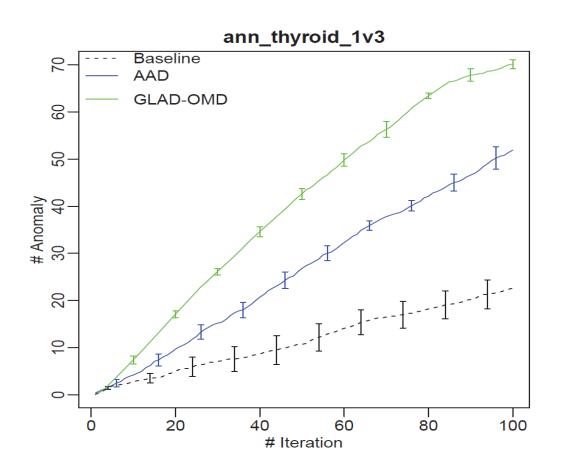
#### **Incorporating User Feedback: Initial Work**

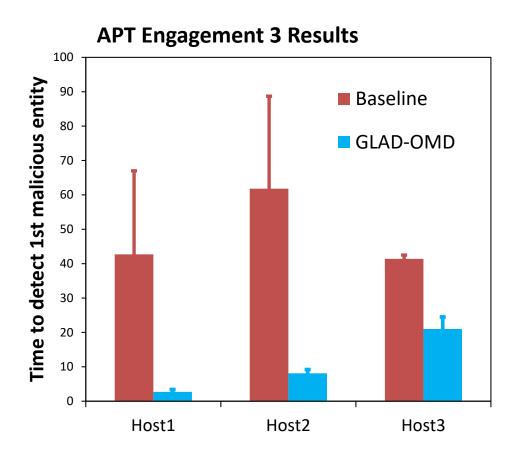
- Show top-ranked candidate to the user
- User labels candidate
- Label is used to update the anomaly detector

[Das, et al, ICDM 2016] GLAD-OMD [Siddiqui, et al., KDD 2018]



# User Feedback Yields Big Improvements in Anomaly Discovery





#### **Explaining Anomalies and Near Misses**

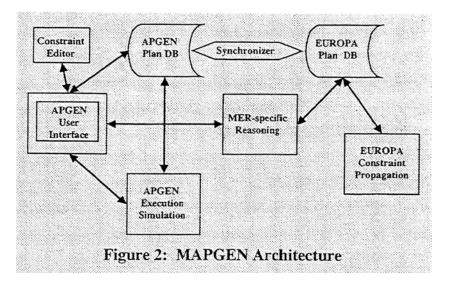
- Existing anomaly explanations are purely statistical
  - "This credit card transaction is anomalous because it was very large compared to this customer's normal behavior"
- Root cause analysis
  - "Customer just purchased a house and is buying furniture for it"
  - Must consider a broader set of hypotheses than in normal state updating
  - May lack dynamics and observation models for this broader space

#### **Improvisational Problem Solving**

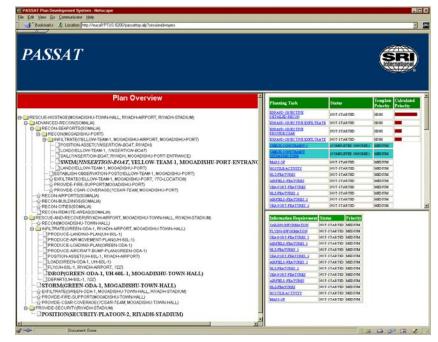
- Human users and AI system collaborate to find solutions
- Humans "think outside the box" to enlarge the problem space
- How can the AI system help humans reason about this larger problem space?
  - Verify that proposed plan does not violate any known system limits or lead to bad system states within the Al's narrow problem space?
  - Can humans communicate the larger space to the AI system so that it can reason about it?
  - Explain to humans how the AI system would behave if permitted autonomy
- Existing work:
  - Mixed-initiative Planning

#### **Mixed-Initiative Planning**

- Agenda of activities that need to be planned
- User-invoked planning operators
  - Plan all: fully automated planning
  - Plan selected goals: incrementally add one or more activities to the emerging plan
  - Expand selected subgoal
  - Create a plan sketch (commit to some activities, possibly at different levels of abstraction)
- User plan editing
  - Move an activity to a different time while disturbing existing steps as little as possible
  - Add/delete activity
  - Delete or relax a constraint
  - Tentatively fix a decision but note that if additional information arrives (e.g., weather forecast) then this decision should be revisited
- System continually checks that all constraints are satisfied and makes changes to satisfy resource constraints and mutual exclusion constraints



MAPGEN: Bresina et al., 2005



#### **Decision Making**

- Person with the relevant expertise should make the final decision
  - Course of action
  - Decision to delegate actions to Al system

#### **Past Failures**

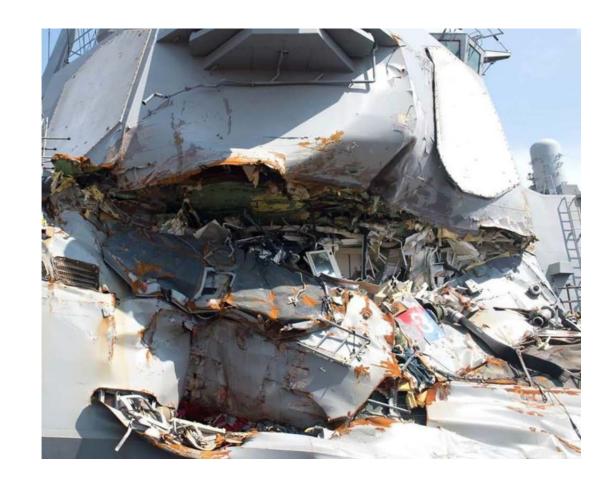
- Al capabilities and limitations are unclear to humans
  - Humans trust Al autonomy when they should not
    - Gulf War Patriot Missile Fratricide
      - New crew operating unfamiliar equipment
      - Broken radio communication with other teams
      - Patriot missile system incorrectly interpreted returning British fighter jet as incoming ballistic missile
      - Crew trusted the system, launched defensive missile: 2 killed
    - Iran-Iraq War AEGIS autonomous ship defense system
      - AEGIS and crew misinterpreted civilian aircraft as incoming attacker despite IFF transponder signal
      - Armed AEGIS which then shot down the aircraft: 290 killed
- Al current and future behavior is difficult for humans to predict
  - Symptom: Humans continually monitor AI system behavior and prepare to intervene at any moment





## Past Failures (2)

- Teamwork failures lead to accidents
  - USS Fitzgerald collision with ACXCrystal
    - Poor communications including failure to use advanced navigation aides led to loss of situational awareness
    - Collision killed 7



#### **Requirements for Human + AI Teams**

- Al System needs to monitor functioning of human team
  - Detect communication failures
  - Detect misunderstandings (failures of shared mental model)
- Al System needs to know when to defer to human expertise
  - Model the expertise of each team member
  - Know whom to engage to obtain information or make a decision
- If human teamwork is breaking down, AI system should abort mission and switch to a safe backup plan

## **Summary: Human + AI Teams**

	Assessment
Situational Awareness	C poor UI, poor communication
Detect Anomalies and Near Misses	C user feedback to anomaly detection
Explain Anomalies and Near Misses	D only basic techniques
Improvise Solutions	D mixed-initiative planning

## **SUMMARY**

#### **Part 1: Trustable Machine Learning**

- Robustness by Construction
  - Budgeted Robust Optimization provides a useful framework
  - Regularization via Stability Training with Noise (STN) provides guarantees and a practical algorithm
- Self-Model of Competence
  - Calibrated Probabilities can be obtained by post-processing classifier scores
  - Classifiers can decide when to reject a query by thresholding calibrated probabilities
- Monitoring for Data Shift
  - Many methods for detecting data shift: anomaly detection, shift in distribution of predicted classes, shift in auxiliary tasks, two-sample test, Old-vs-New classifier test

#### Part 2: Robust Al Systems

- High Reliability Human Organizations provide a model for achieving robustness in complex, safetycritical tasks
- Part 2A: Autonomous Al Systems
  - Maintain Situational Awareness (well understood)
  - Detecting Anomalies and Near Misses (many open questions)
  - Explaining Anomalies and Near Misses (virtually no research yet)
  - Improvising Solutions (essentially no research yet)
- Part 2B: Combined AI + Human Teams
  - Maintain Situational Awareness (past systems had very poor situational awareness)
    - Opportunity: Transparent UI to help users achieve appropriate trust
    - Need: Joint human-Al situational awareness
  - Detecting Anomalies and Near Misses (need methods that encompass the human team and other agents)
    - Opportunity: Interactive Anomaly Detection
  - Explaining Anomalies and Near Misses (beyond explainable AI for classifiers)
  - Improvising Solutions (AI needs to support and extend human improvisation)

#### **Guideline for Deploying AI in High Risk Situations**

- We should only apply AI in high-risk situations when we can create and maintain a high-reliability organization that combines the human and AI systems
  - Al system must support and perform the five functions of HROs
- Examples to consider:
  - Face Recognition in Law Enforcement
    - Searches against face databases vs. Real-time Body Cam identification?
  - Self-Driving Cars
    - No. A human driver can't be an HRO. Al must be fully autonomous
  - Al Trading Systems
    - Currently lack anomaly detection, joint situational awareness. Operate too quickly for human intervention
  - Autonomous Weapons Systems
    - Maybe: Military teams already train to be HROs. But AI capabilities still lacking

## **QUESTIONS?**